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k -Cycle resonant graphs[☆]

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Abstract

A connected graph G is said to be k -cycle resonant if, for $1 \leq t \leq k$, any t disjoint cycles in G are mutually resonant, that is, there is a perfect matching M of G such that each of the t cycles is an M -alternating cycle. In this paper, we at the first time introduce the concept of k -cycle resonant graphs, and investigate some properties of k -cycle resonant graphs. Some simple necessary and sufficient conditions for a graph to be k -cycle resonant are given. The construction of k -cycle resonant hexagonal systems are also characterized.

1. Introduction

In the investigation of the graphs with perfect matchings, many special classes of graphs have been introduced, such as elementary graphs, 1-extendable (or matching covered) graphs, n -extendable graphs, saturated graphs, factor-critical and bicritical graphs, etc. [1–9]. The properties and constructions of these classes of graphs have been also investigated extensively. In Ref. [1], Lovász and Plummer summarized works on these topics.

Let G be a graph with perfect matchings. An edge of G is said to be allowed if it lies in a perfect matching of G , otherwise forbidden. A graph G is said to be elementary if its allowed edges form a connected subgraph of G . An elementary graph G is said to be 1-extendable (or matching covered) if all of its edges are allowed. In the topological theory of benzenoid hydrocarbons, mathematic chemists [10–14] are interested in normal hexagonal systems, which just correspond to 1-extendable polyhex graphs. A hexagonal system H is a 2-connected finite subgraph in the hexagonal lattice such that every interior face of H is bounded by a hexagon. A perfect matchings of a hexagonal system H is also called a Kekulé structure by chemists. For a Kekulé

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structure M of H , an edge in M is called an M -double bond, otherwise an M -single bond. An edge of H is said to be a fixed double (single) bond of H if it is always a double (single) bond in every Kekulé structure of H .

A normal hexagonal system is a hexagonal system with no fixed bond. Zhang Fuji and Chen Rongsi [13] proved that a hexagonal system H is normal if and only if every hexagon of H is resonant, that is, for any hexagon s of H , there is a Kekulé structure M of H such that s is an M -alternating cycle. A normal hexagonal system is also said to be 1-coverable. The concept of k -coverable hexagonal systems was introduced by Zheng Maolin [14]. A hexagonal system H is said to be k -coverable if H contains at least k disjoint hexagons and, for $1 \leq t \leq k$, any t disjoint hexagons of H are mutually resonant, that is, there is a Kekulé structure M such that the t disjoint hexagons are M -alternating cycles. The properties and construction of k -coverable hexagonal systems have been also investigated by the same author.

In the present paper, we are going to introduce a new class of graphs with perfect matchings, called k -cycle resonant graphs or k -cycle extendable graphs, which are a natural generalization of k -coverable hexagonal systems and n -extendable graphs. Some simple necessary and sufficient conditions for a graph to be k -cycle resonant are given. The construction of k -cycle resonant hexagonal systems are characterized.

It should be mentioned that the concept of conjugated circuits (namely, resonant cycles) in hexagonal systems was first introduced by Randić [15]. Enumeration of conjugated circuits has led to expressions for the resonant energies of polycyclic conjugated hydrocarbons, etc. Furthermore, Gutman and Randić [16] extended enumeration of conjugated circuits to include disjoint conjugated circuits. The k -cycle resonant graphs we introduce here have the property that, for $1 \leq t \leq k$, any t disjoint cycles are mutually resonant (or conjugated).

2. k -Cycle resonant graphs

Definition 2.1. Let G be a connected graph with perfect matchings. G is said to be k -cycle resonant (or extendable) if G contains at least k (≥ 1) disjoint cycles and, for $1 \leq t \leq k$, any t disjoint cycles in G are mutually resonant, that is, there is a perfect matching M of G such that the t disjoint cycles are M -alternating cycles.

Let G be a connected graph. Let G_i be a vertex-induced subgraph of G . For convenience, we denote by $G - G_i$ the graph obtained from G by deleting the vertices in G_i and their incident edges. A maximal 2-connected subgraph in G is called a 2-connected component of G . For a connected graph G with perfect matchings, an edge e of G is said to be a fixed double (single) bond if e belongs (does not belong) to any perfect matching of G . For a 2-connected graph G , a path P in G is said to be a chain if the degree of any end vertex of P is greater than two and the degree of any middle vertex of P is equal to two in G . A chain P in a 2-connected graph G is said to

be a reducible chain if $G - V_m(P)$ is 2-connected, where $V_m(P)$ is the set of middle vertices of P ; otherwise irreducible.

Theorem 2.2. *Let G be a k -cycle resonant graph. Then*

- (1) G is bipartite.
- (2) For $1 \leq t \leq k$ and any t disjoint cycles C_1, C_2, \dots, C_t in G , $G - \bigcup_1^t C_i$ contains no odd component.
- (3) Any two 2-connected components in G have no common vertex.

Proof. (1) and (2) hold obviously.

(3) Suppose that G_i, G_j are two 2-connected components in G , which have a common vertex v . Then v is a cut vertex of G . Let G'_i be the component of $G - v$ which contains $G_i - v$, and let C_j be a cycle in G_j which contains v . Since C_j is resonant in G , G'_i must be an even component in $G - C_j$. For a cycle C_i in G_i , which contains v , the number of the vertices in $V(G'_i) \cap V(C_i)$ is odd, and so is $|V(G'_i) \setminus V(C_i)|$, implying that $G - C_i$ contains an odd component, that is, C_i is not resonant in G . This contradicts that G is k -cycle resonant. \square

Theorem 2.3. *Let G be a k -cycle resonant graph. Then G is elementary or 1-extendable if and only if G is 2-connected.*

Proof. If G is not 2-connected, by Theorem 2.2 (3), G must contain cut edges. Clearly, any cut edge of G must be a fixed bond (double or single), implying that G is not elementary and 1-extendable.

If G is 2-connected, then any edge e of G is contained in a cycle of G [17], and the cycle is a resonant cycle. So e is not a fixed bond, implying that G is 1-extendable and elementary. \square

From the above theorems and Theorem 4.1.1 in Ref. [1], we have the following corollary.

Corollary 2.4. *Let G be a 2-connected k -cycle resonant graph with bipartition (U, W) . Then*

- (1) G has exactly two minimum vertex covers, namely U and W .
- (2) For every nonempty proper subset X of U , $N(X) \geq |X| + 1$, where $N(X)$ denotes the neighbour set of X .
- (3) If $|U| = |W| \geq 2$, for any $u \in U, w \in W$, $G - u - w$ has a perfect matching.

Theorem 2.5. *Let G be a 2-connected k -cycle resonant graph. Then any reducible chain of G is of odd length.*

Proof. Let P be a reducible chain of G .

Since $G - V_m(p)$ is 2-connected, there is a cycle C in $G - V_m(p)$ passing through two end vertices of p . The component in $G - C$ induced by $V_m(p)$ must be an even component, since C is resonant. So P is of odd length. \square

3. Some necessary and sufficient conditions for a graph to be k -cycle resonant

Theorem 2.2(1), (2) give some necessary conditions for a graph to be k -cycle resonant. We can prove these necessary conditions are also sufficient.

Theorem 3.1. *A connected graph with at least k disjoint cycles is k -cycle resonant if and only if G is bipartite and, for $1 \leq t \leq k$ and any t disjoint cycles C_1, C_2, \dots, C_t in G , $G - \bigcup_1^t C_i$ contains no odd component.*

Proof. We need only to prove the sufficiency.

For $k = 1$, let G be bipartite, and let $G - C$ contains no odd component for any cycle C in G .

Suppose that G is not 1-cycle resonant. Then there is a cycle C^* in G , such that $G - C^*$ has a component with no perfect matching, say G^* . Without loss of generality, we choose G^* such that G^* is minimal in the above sense.

Let v_1, v_2, \dots, v_m be the vertices on C^* each of which is adjacent to a vertex in G^* , and they divide C^* into m edge-disjoint segments $v_1 - v_2, v_2 - v_3, \dots, v_i - v_{i+1}, \dots, v_m v_1$. Since G^* is connected, there is a path $P(v_i, v_{i+1})$, starting from v_i , passing through some vertices in G^* , and terminating in v_{i+1} . Let C' be the cycle consisting of $P(v_i, v_{i+1})$ and the segment $v_{i+1} - v_{i+2} - \dots - v_i$ on C^* . Then $|V(P(v_i, v_{i+1})) \cap V(G^*)|$ must be an even number. Otherwise $G^* - V(P(v_i, v_{i+1}))$ would contain an odd component which is also an odd component of $G - C'$, contradicting our assumption. Then $G^* - V_m(P(v_i, v_{i+1}))$ must have no perfect matching. Otherwise, G^* would have a perfect matching, a contradiction. Hence $G^* - V_m(P(v_i, v_{i+1}))$ contains a component with no perfect matching, say G^{**} , which is also a component of $G - C'$. But G^{**} is a proper subgraph of G^* , contradicting the choice of G^* .

We now assume that the conclusion of the theorem holds for $k \leq n$. Let $k = n + 1$.

Then G is bipartite, and, for $1 \leq t \leq n + 1$ and any t disjoint cycles C_1, C_2, \dots, C_t in G , $G - \bigcup_1^t C_i$ contains no odd component.

If $t \leq n$, by the induction hypothesis, G is t -cycle resonant.

If $t = n + 1$, for any $n + 1$ disjoint cycles $C_1, C_2, \dots, C_n, C_{n+1}$ in G , $G - \bigcup_1^n C_i$ has a perfect matching, since G is n -cycle resonant. Then the component G_{n+1} in $G - \bigcup_1^n C_i$ which contains C_{n+1} satisfies that G_{n+1} is bipartite, and, for any cycle C'_{n+1} in G_{n+1} , $G_{n+1} - C'_{n+1}$ contains no odd component. So G_{n+1} is 1-cycle resonant, implying that $C_1, C_2, \dots, C_n, C_{n+1}$ are mutually resonant, and so G is $(n + 1)$ -cycle resonant. \square

4. k -cycle resonant hexagonal systems

A hexagonal system H is a 2-connected plane graph whose every interior face is bounded by a regular hexagon. If H contains no interior vertex, it is said to be a catacondensed hexagonal system, otherwise a pericondensed hexagonal system. For k -cycle resonant hexagonal systems, we can give a more explicit construction characterization.

Theorem 4.1. *A hexagonal system H is 1-cycle resonant if and only if H is a catacondensed hexagonal system.*

Proof. Suppose that H is 1-cycle resonant, but H not a catacondensed hexagonal system. Then in H there is a subsystem H' which is a pericondensed hexagonal system with only three hexagons. Let C be the boundary of H' . In the interior of the cycle C there is only one interior vertex of H , which is an odd component in $H - C$, contradicting that H is 1-cycle resonant.

Conversely, suppose that H is a catacondensed hexagonal system.

For any cycle C in H , let $H(C)$ be the subsystem of H whose boundary is C , and let $G(C)$ be the graph induced by the hexagons in the exterior of C . Then $H(C)$ and any component H_i of $G(C)$ are also catacondensed hexagonal systems, and H_i and C have exactly one common edge. So $H - C$ contains no odd component. Now it follows from Theorem 3.1 that H is 1-cycle resonant. \square

Theorem 4.2. *A hexagonal system H is 2-cycle resonant if and only if (1) H contains at least two disjoint hexagons, and (2) H is a catacondensed hexagonal system with no chain of even length.*

Proof. Suppose that H is 2-cycle resonant. By Theorems 4.1 and 2.5, H is a catacondensed hexagonal system, and any reducible chain of H is of odd length. For an irreducible chain P of H and the end vertices u_1, u_2 of P , there are two disjoint hexagons in $H - V_m(P)$, say s_1, s_2 , such that s_1 contains u_1 and s_2 contains u_2 . Since s_1, s_2 are mutually resonant, $P - u_1 - u_2$ is an even component in $H - s_1 - s_2$, implying that P is of odd length.

Conversely, suppose that H satisfies conditions (1) and (2) in the theorem, but H is not 2-cycle resonant. Then there are two disjoint cycles C_i, C_j such that $H - C_i - C_j$ contains an odd component G_0 , by Theorem 3.1. Every 2-connected component in G_0 is a catacondensed hexagonal system. After deleting all 2-connected components of G_0 , the remains contain an odd component which is a path of even length, say P' . Every end vertex of P' is just adjacent to one vertex of degree three in H . Let the two vertices of degree three are u_1, u_2 . Then $V(P') \cup \{u_1, u_2\}$ induces a chain of even length in H , contradicting our assumption. \square

Theorem 4.3. Let H be a 2-cycle resonant hexagonal system, and let k^* be the maximum number of disjoint cycles in H . Then H is k^* -cycle resonant.

Proof. By Theorem 4.2, H is a catacondensed hexagonal system with no chain of even length. Suppose that H is k -cycle resonant, but not $(k+1)$ -cycle resonant for $2 \leq k < k^*$. Then there are $k+1$ disjoint cycles C_1, C_2, \dots, C_{k+1} such that $H - \bigcup_{i=1}^{k+1} C_i$ contains an odd component. By the same reason as in the proof of Theorem 4.2, a chain of even length in H would be found, a contradiction. \square

From Theorems 4.2 and 4.3, we have the following theorem.

Theorem 4.4. A hexagonal system H is k^* -cycle resonant if and only if H is a catacondensed hexagonal system with no chain of even length, where k^* is the maximum number of disjoint cycles in H .

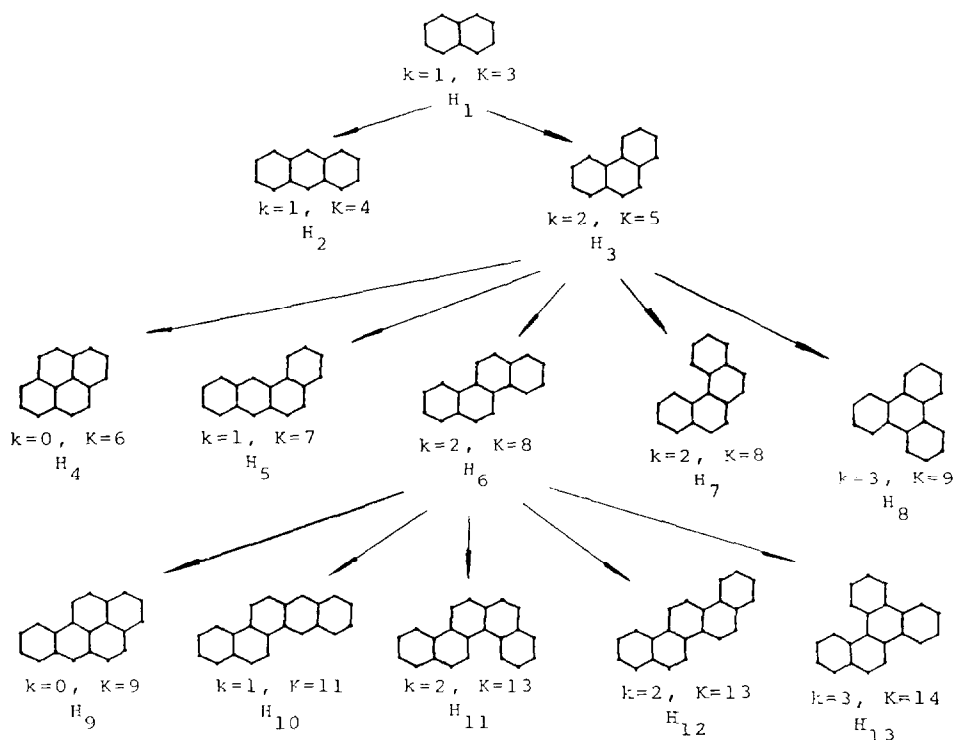


Fig. 1. Some hexagonal systems with h hexagons obtained from a same parent hexagonal system with $h-1$ hexagons, where k indicated that the corresponding hexagonal system is k -cycle resonant and K is the number of Kekulé structures.

Table 1. The resonance energies of the hexagonal systems as shown in Fig. 1, where RE(LM) denotes the resonance energy based on the logarithmic model and RE denotes the resonance energy based on conjugated circuit model

| Hexagonal system | k | K | RE(LM) (eV) | RE (eV) |
|------------------|-----|-----|-------------|---------|
| H_1 | 1 | 3 | 1.3020 | 1.3233 |
| H_2 | 1 | 4 | 1.6422 | 1.5998 |
| H_3 | 2 | 5 | 1.9068 | 1.9552 |
| H_4 | 0 | 6 | 2.1232 | 2.1332 |
| H_5 | 1 | 7 | 2.3058 | 2.3107 |
| H_6 | 2 | 8 | 2.4642 | 2.5058 |
| H_7 | 2 | 8 | 2.4642 | 2.5058 |
| H_8 | 3 | 9 | 2.6046 | 2.7078 |
| H_9 | 0 | 9 | 2.6040 | 2.5850 |
| H_{10} | 1 | 11 | 2.8424 | 2.8279 |
| H_{11} | 2 | 13 | 3.0404 | 3.0916 |
| H_{12} | 2 | 13 | 3.0404 | 3.0916 |
| H_{13} | 3 | 14 | 3.1273 | 3.2082 |

5. Conclusion

The present work establishes some simple necessary and sufficient conditions for a graph to be k -cycle resonant, which are a good characterization in Edmonds' sense [18]. By using the conditions, the construction of k -cycle resonant hexagonal systems is completely characterized. It may be interesting for chemists that, in the hexagonal systems with h hexagons obtained from a same parent hexagonal system with $h-1$ hexagons, k^* -cycle resonant systems have greater resonance energies than 1-cycle resonant systems, also 1-cycle resonant systems have greater resonance energies than hexagonal systems not being 1-cycle resonant. This is true for the logarithmic model [19–21] and the Randić's conjugated circuit model [15, 22–29] (see Fig. 1 and accompanying Table 1). One also finds that the number of cycles in a proper Clar formula [30] of a k^* -cycle resonant hexagonal system is just equal to k^* .

For general k -cycle resonant graphs, the construction of them are more complex. We shall discuss it elsewhere.

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